

2,2,2-Trifluoroethanol
75-89-8 | DTXSID0021751

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 56.4 mmHg

Global applicability domain: Inside

Local applicability domain index: 7.05e-01

Confidence level: 7.22e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Chloral</div> <div>Measured: 71.3</div> <div>Predicted: 41.1</div>	<div>Image not found</div> <div>Camphor</div> <div>Measured: 14.7</div> <div>Predicted: 3.22e-01</div>	<div>Image not found</div> <div>D-Camphor</div> <div>Measured: 14.7</div> <div>Predicted: 3.22e-01</div>
<div>Image not found</div> <div>Ethylene sulfide</div> <div>Measured: 46.1</div> <div>Predicted: 166</div>	<div>Image not found</div> <div>Cyclohexane, dodecafluoro-</div> <div>Measured: 60.9</div> <div>Predicted: 141</div>	<div>Image not found</div> <div>Hexanal</div> <div>Measured: 127</div> <div>Predicted: 18.2</div>